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by

Roger A. Strehlow

Approved for public release; distribution unlimited

Grant No. AFOSR 77-3336 December 1979

Interim Technical Report

ENGINEERING EXPERIMENT STATION, COLLEGE OF ENGINEERING, UNIVERSITY OF ILLINOIS, URBANA

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Simple acoustic source theory has been applied to determine the maximum overpressure obtainable by the deflagration of nonspherical clouds. In three dimensions overpressure is generated not by the rate of energy addition but by the first time derivative of the rate. Because of this, deflagrative combustion of edge-ignited clouds produces markedly less overpressure than central, spherical ignition. Examples are presented for three nonspherical cloud and igniter geometries. The implication is that even high velocity, → over page

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ABSTRACT

Simple acoustic source theory has been applied to determine the maximum overpressure obtainable by the deflagration of non-spherical clouds. In three dimensions overpressure is generated not by the rate of energy addition but by the first time derivative of the rate. Because of this, deflagrative combustion of edge-ignited clouds produces markedly less overpressure than central, spherical ignition. Examples are presented for three non-spherical cloud and igniter geometries. The implication is that even high velocity, subsonic combustion waves cannot produce damaging blast waves and that some type of supersonic combustion or massive flame acceleration is required if a damaging blast wave is to be produced.

INTRODUCTION

The determination of the blast wave produced in free space by the nonspherical combustion of a nonspherical vapor cloud has not been examined in any detail, either analytically or numerically. The problem is important because at the present time spherical theory is being used to estimate the overpressure for clouds of arbitrary shape and no one knows how conservative this approach is. This paper applies simple acoustic source theory to the deflagrative combustion of a few simple free cloud shapes to determine a first cut estimate of the maximum overpressure that one could expect as a function of cloud size and shape.

THE SIMPLE ACOUSTIC SOURCE

Stokes[1] first showed that a simple source of mass at a point $\dot{m}(t)$ (Units: Kg/sec) generates a sound wave in three dimensions which has an overpressure which is proportional to $\ddot{m}(t)$. Specifically, as Lighthill[2] states,

$$P - P_o = \ddot{m}\left(t - \frac{r}{a_o}\right)/4\pi r \qquad (1)$$

where $t - \frac{r}{a_o}$ replaces t because the wave is propagating away from the source region at the velocity of sound, a_o. Lighthill also states that at some distance from the source the sound will appear to emanate from a point (i.e., the wave will be very close to spherical) if the quantity $(\omega r/a_o)^2 << 1$. Here, ω is the circular

frequency of the source of sound and r is a characteristic radius of the source region. Finally, for a source which has a finite duration $\int\ddot{m}(t)dt = 0$, and therefore $\int(P-P_o)dt = 0$ in the wave. This means that the acoustic pulse from a source of finite duration must have a negative phase impulse equal to the positive phase impulse. This should be contrasted to the pulse emitted by a finite duration source in a strictly one-dimensional channel. In this case the acoustic overpressure is proportional to $\dot{m}(t)$ and the overpressure in the pulse is always positive everywhere.[1]

Now consider the deflagrative combustion of an unconfined cloud of arbitrary shape. For simple source acoustic behavior the effective rate of mass addition $\dot{m}(t)$ may be replaced by an effective rate of volume addition multiplied by the initial gas density, that is, $\dot{m}(t) = \rho_o\dot{v}(t)$.

However, for deflagrative combustion

$$\dot{m}(t) = \rho_o\dot{v}(t) = \rho_o\left(\frac{V_b - V_u}{V_u}\right)\frac{d}{dt}\left(S_u(t) \cdot A_f(t)\right) \tag{2}$$

where $S_u(t)$ is the effective normal burning velocity, $A_f(t)$ is the effective frontal area of the flame and the ratio $(V_b-V_u)/V_u$ is the new volume produced per unit volume of gas burned at constant pressure. Using the notation of Strehlow et al.[3] $(V_b-V_u)/V_u = \hat{q}/\gamma_o$. Here, $\hat{q}$ is an effective dimensionless heat addition. Its relation to the $\tilde{q}$ of Strehlow et al. is given in Appendix A. Therefore, using the definition of the velocity of sound in an ideal gas and

combining Eqs. (1) and (2) yields

$$\overline{P} = \frac{\hat{q}}{4\pi a_o^2 r} \frac{d}{dt} [S_u(t) \cdot A_f(t)]$$

where $\overline{P}$ is the acoustic overpressure. Equation (3) is a significant relationship. It states that the acoustic overpressure generated by deflagrative combustion in three dimensions is given by the <u>time</u> <u>rate</u> <u>of</u> <u>change</u> of the <u>rate</u> of energy addition rather than the rate of energy addition as it is in strictly one-D flow.

The deflagrative combustion of a cloud generates a sound wave of very low frequency. The period of the sound source in this case is given by $\tau = 2\pi/\omega$ where τ is the burn time. Thus the requirement that the source region is acoustically simple becomes

$$[2\pi(r_m/\tau)/a_o]^2 << 1$$

where r_m is a major dimension of the cloud and approximates the distance traversed by the deflagration wave. Even with distortion and motion due to flame propagation $r/\tau \simeq S_u$ and the simple source requirement becomes $4\pi^2 M_{Su}^2 << 1$. If the quantity is to be less than 0.1 for no blast wave distortion S_u will be about 17.5 m/sec before deflagrative behavior produces significant distortion of the blast wave. Even for significantly higher values of S_u the first effect will be only to distort the shape of the blast wave. Higher overpressures than estimated here will not occur until S_u becomes quite large. This limitation of the theory has not been quantified as yet.

APPLICATION IN SPHERICAL GEOMETRY

Two classical problems have been treated in spherical geometry. These are the centrally-ignited, constant-velocity flame[3,4] and the Taylor piston problem.[5] For a constant-velocity flame Eq. (3) reduces to the relation

$$\overline{P} = \frac{\hat{q}S_u}{4\pi a_o^2 r}\frac{dA_f}{dt} \tag{4}$$

where r is the distance from the source to the observer. For a growing spherical flame ball

$$A_f = 4\pi r_f^2$$

and

$$\frac{dr_f}{dt} = S_S = S_u \frac{V_b}{V_u}$$

Substituting yields

$$\overline{P} = \frac{2\hat{q}S_u^2 r_f}{a_o^2 r}\left(\frac{V_b}{V_u}\right)$$

where the r in the denominator must be equal to or greater than r_f. If we let it be equal to r_f, and if we substitute the definition of $\hat{q}$ given above, we obtain an expression for the acoustic pressure on the unburned side of the flame

$$\overline{P}_f = 2\gamma\left(1 - \frac{V_u}{V_b}\right)\left(\frac{V_b}{V_u}\right)^2 M_{Su}^2 \tag{6}$$

which is identical to Eq. (19) of Strehlow et al.[3]

If we write $r_f = S_S t$ for the flame propagation in Eq. (5) and recall that away from the flame t becomes $\left(t - \frac{r}{a_o}\right)$ Eq. (5) may be written

$$\overline{P} = 2\gamma\left(1 - \frac{V_u}{V_b}\right)\left(\frac{V_b}{V_u}\right)^3 M^3_{Su} \left(\frac{a_o t}{r} - 1\right) \tag{7}$$

However, the transformation from a flame to a Taylor spherical piston is

$$M_p = \left(1 - \frac{V_u}{V_b}\right)^{1/3} \frac{V_u}{V_b} M_{Su}$$

Therefore, Eq. (7) reduces to

$$\overline{P} = 2\gamma_o M^3_p\left(\frac{a_o t}{r} - 1\right) \tag{8}$$

where the range on r is $S_p t < r < a_o t$. Equation (8) is identical to the Taylor solution for a spherical piston as $M_p \to 0$ (Eq. (13), Strehlow et al.[3]).

We note that in these equations the rate of flame area growth is proportional to r and the rate of decay of a spherical acoustic pulse is proportional to r^{-1}. Thus, for the spherical case the acoustic pressure remains constant at the flame front and the wave that is generated during flame motion is self-similar in r/t. This is a fundamental acoustic property of a constant-velocity flame that is completely surrounded by combustible material when it burns. It has been verified by numerous theoretical and numerical investigations.[3,4]

APPLICATION TO FREE CLOUDS

We restrict ourselves to clouds of arbitrary shape in free space. To simplify the treatment, we will consider free clouds which have a horizontal plane of symmetry for cloud shape, cloud distortion during deflagration and deflagration wave shape. Since we now wish to simply examine the implications of Eq. (3) for general geometries, we for the moment restrict ourselves to considering only constant velocity flames. This means that Eq. (3) reduces to Eq. (4) where S_u is an effective normal burning velocity and r is the distance of an observer from the cloud center.

In general the evaluation of the dA_f/dt term in Eq. (4) is complicated because during deflagrative combustion the cloud ahead of the flame will move and distort with time. This distortion will cause A_f to be a different function of time than that calculated from purely geometric considerations using a constant velocity flame propagating through a stationary cloud.

In order to determine how to best approximate the effect of such distortion for arbitrary ignition of an arbitrary cloud one must first examine flow behavior in two simple limit geometries; strictly one-dimensional flow caused by deflagration and volumetric heat addition in three dimensions.

The wave diagram for a strictly one-D flow driven by a constant-velocity deflagration wave is shown in Fig. 1. If we model the combustion of a stoichiometric methane-air mixture as proposed in Strehlow et al.,[3] the gas to the right of the flame and to the

left of the contact surface (regions 0, 1 & 3) can be assumed to have a heat capacity ratio $\gamma_0 = \gamma_1 = \gamma_3 = 1.4$, while the gas in region 2 has a $\gamma_2 = 1.202$. Additionally, the effective value of dimensionless energy addition is $\tilde{q} = 8.430$. This means (from Appendix A) that $\hat{q} = 9.242$ and that $V_b/V_u = 7.602$ for constant pressure combustion. Furthermore, for this system the Chapman-Jouguet deflagration Mach number is 0.16631.

The properties of the wave system of Fig. 1 were calculated using the shock relationships from Liepman and Roshko[6] for the shocks S_1 and S_3, the deflagration relationship from Strehlow et al.[3] for the flame and the contact surface requirement that $U_{p_2} = U_{p_3}$ and $P_2 = P_3$. The results of this calculation that are important to this paper are summarized in Fig. 2.

Figure 2 shows that particle velocities generated by flame propagation are relatively high and that the apparent flame speed relative to an observer is from 4.3 to 9.3 times the actual normal burning velocity. Also it is less than the space velocity of a spherical flame if the one-dimensional flame is traveling at less than about 0.9 of its maximum (CJ) velocity. Furthermore, the ratio $|U_{p_3}/U_{p_1}|$ lies between 1.0 and 1.4 in this same velocity range. This last observation simply means that even relatively high speed flame propagation from a free surface in one-dimensional space displaces the gas rather uniformly to the front and back. This is to be contrasted to the behavior of a one-dimensional CJ detonation, which displaces the gas primarily in the direction of detonation propagation.

We now wish to determine what happens if we relax the confinement normal to the flame propagation direction for the case of deflagrative combustion. To estimate this effect we assume that if energy is added relatively slowly to a gaseous volume, the volume will expand an equal distance in all directions. During flame propagation through a cloud the flame can be assumed to be a relatively thin sheet of energy addition when compared to the cloud dimensions. In other words the flame can be assumed to occupy a volume $A\Delta L$ when $\Delta L << \sqrt{A}$. Under these circumstances one would expect the major expansion to occur in a direction normal to the local orientation of the flame even though the pressure is propagating almost equally in all three dimensions.

This assumption has been qualitatively verified experimentally by observing flame propagation in a propane-air elongated pancake cloud above a flat plate of about 50 mm height and 0.6 m x 0.3 m, edge ignited at the center of the 0.3 m edge.(7) The flame's apparent propagation speed was about 3.5 times the normal burning velocity, and its luminous height was about equal to the initial cloud height. Furthermore the flame flashed to encompass an area considerably larger than the original lateral extent of the cloud. The assumption has also been reasonably well verified by numerical calculations made by Dr. Len Hazelman(8) at Lawrence Livermore Laboratories using a 2 D hydrocode. He calculated flow and flame propagation in an open 2 D channel. His calculations yielded a flame height almost twice the initial cloud height and an

apparent flame speed about three times the normal burning velocity. However, his numerical flame had a thickness only one-third of the cloud height and this should lead to more vertical distortion.

These results indicate that for any arbitrary free cloud and igniter geometry in which the flame is not completely surrounded by a combustible mixture one may make the following conservative assumptions about flame-induced distortion.

1. The burning velocity that should be used is S_u. This is because, irrespective of the motion of the flame induced by the flow, the entire cloud will burn in a time, τ, given by $S_u\tau = r_m$ where r_m is the distance from the igniter to the farthest point in the initially quiescent cloud.

2. The increase of flame area in a free cloud due to distortion of the cloud by flame-induced flow will never exceed the value V_b/V_u calculated for isoboric combustion. This is because this is the value of distortion of the unburned material produced during combustion of a completely surrounded (spherical) flame, and relief due to product gas motion away from the flame can only reduce this factor.

Thus the general procedure for determining a first conservative approximation to the effect of cloud shape and igniter location on the overpressure-time behavior in the blast wave when the igniter is not completely surrounded by the cloud is as follows:

1. Assume a value of S_u.

2. Assume a cloud geometry and igniter location.
3. Calculate dA_f/dt for a flame traveling at velocity S_u through the quiescent cloud.
4. Correct for distortion by multiplying by V_b/V_u.

<u>Examples for Specific Geometries</u>

a. Central (line) ignition of a pancake cloud.

The flame area is given by

$$A_f = 2\pi r_f H$$

where r_f is the flame radius and H is the height of the pancake. Therefore

$$\frac{dA_f}{dt} = 2\pi H \frac{dr_f}{dt} = 2\pi H S_u$$

and

$$\overline{P}_{max} = \frac{\rho S_u^2 H}{2a_o^2 R_{obs}} \left[\frac{V_b}{V_u}\right] \qquad (9)$$

where R_{obs} is the distance of an observer from the center of the cloud.

b. Edge (line) ignition of a pancake cloud.

The area of a flame propagating from an edge of a cloud of radius R is given in terms of the distance propagated by the formula

$$A_f = 2Hr_f \cos^{-1} \frac{r_f}{2R} \quad .$$

Now

$$\frac{dA_f}{dt} = \frac{dA_f}{dr_f} \cdot \frac{dr_f}{dt} = \frac{dA_f}{dr_f} \cdot S_u$$

Therefore

$$\overline{P} = \frac{\hat{q}S_u^2H}{2\pi a_o^2 r}\left[\cos^{-1}\frac{r}{2R} - \frac{\frac{r}{2R}}{\sqrt{1-\left(\frac{r}{2R}\right)^2}}\right]\left(\frac{V_b}{V_u}\right)$$

or

$$\overline{P}_{max} = \frac{\hat{q}S_u^2H}{4a_o^2R_{obs}}\left(\frac{V_b}{V_u}\right) \qquad (10)$$

which is exactly half that predicted for a centrally-ignited pancake.

c. End (point) ignition of an ellipsoid (cigar-shaped) cloud.

Assume a flat flame of location r_f propagates from one end of a long cloud with a minor radius of rotation d and major radius b.

Flame area is therefore

$$A_f = \pi d^2\left[1 - \frac{r_f^2}{b^2}\right]$$

or

$$dA_f = -\,2\pi r_f \frac{d^2}{b^2}$$

Now let

$$-\,b = -\,L/2 \le r \le L/2 = b \qquad \text{and} \qquad D = 2d$$

where L is the length of the ellipsoid.

Therefore

$$\overline{P} = \frac{-\hat{q}S_u^2D^2}{2a_o^2rL^2}\, r_f \left(\frac{V_b}{V_u}\right)$$

and

$$\overline{P}_{max} = \frac{\hat{q}S_u^2}{4a_o^2} \cdot \frac{D}{R_{obs}} \cdot \frac{D}{L}\left(\frac{V_b}{V_u}\right) \tag{11}$$

Now assume that $\hat{q}$, S_u, a_o and (V_b/V_u) are independent of cloud shape and that the observer is at a fixed distance from the center of a cloud of fixed volume but of these different shapes. Call the volumes $V_s = V_p = V_c$, where the subscripts s, p and c refer to spherical, pancake and cigar shaped clouds, respectively. Also define the aspect ratio of the cloud $\mathcal{R}$ as $\mathcal{R}_p = 2R_p/H_p$ and $\mathcal{R}_c = D_c/L_c$. Using this notation we obtain

$$H_p = D\sqrt[3]{\frac{2}{3\,\mathcal{R}^2}} \tag{12}$$

and

$$D_c = \frac{D_s}{\sqrt[3]{\mathcal{R}}} \tag{13}$$

Combining Eqs. (5), (9), (10) and (11) with Eqs. (12) and (13) yields

$$\left(\frac{\overline{P}_p}{\overline{P}_s}\right)_{max} = \frac{1}{\left[12\left(\frac{\hat{q}}{\gamma_o} + 1\right)\mathcal{R}^2\right]^{1/3}} \tag{14}$$

and

$$\left(\frac{\overline{P}_c}{\overline{P}_s}\right)_{max} = \left[\frac{2}{3\left(\frac{\hat{q}}{\gamma_o} + 1\right) \mathit{AR}^{4}}\right]^{1/3} \tag{15}$$

where the factor $\frac{\hat{q}}{\gamma_o} + 1 = V_b/V_u$ arises because we are considering the initial cloud diameter and Eq. (5) is written in terms of the final radius. Eq. (14) is for central-line ignition of a pancake: for edge-line ignition $(\overline{P}_c/\overline{P}_s)_{max}$ is one half of this value.

Figure 3 is a plot of Eqs. (13) and (14). It shows that the deflagration, after edge ignition of a large aspect-ratio cloud, produces much lower overpressures than central ignition of a spherical cloud. It should be pointed out that point ignition of the edge of a free spherical cloud $\mathit{AR}_c = 1$ would yield a higher overpressure than calculated with Eq. (14) because the derivation of Eq. (11) assumed a flat flame. In reality one would expect a flame of roughly spherical shape to propagate away from a point source and the initial rate of flame area increase would be larger in this case than for a flat flame.

EFFECT OF CLOUD SIZE

Equation (3) can be used to give an order of magnitude estimate of flame areas and accelerations that are necessary for a deflagration to produce a damaging blast wave. If we define the threshold of damage to be 0.1 Bar and assume that this level of overpressure is to be produced 100 m from the cloud center in an atmosphere with a velocity of sound of 350 m/s, Eq. (3) reduces to

$$1.6 \times 10^7 = A_f \frac{dS_u}{dt} + S_u \frac{dA_f}{dt} \tag{16}$$

Table I was constructed from Eq. (16) under the two limit assumptions that (1) $dS_u/dt = 0$ and (2) $dA_f/dt = 0$.

TABLE I

(1) $dS_u/dt = 0$		(2) $dA_f/dt = 0$	
S_u, m/s	$\frac{dA_f}{dt}$, m^2/s	A_f, m^2	$\frac{dS_u}{dt}$, m/s^2
1	1.7×10^7	100	1.7×10^5
10	1.7×10^6	10,000	1.7×10^3
100	1.7×10^5	1,000,000	17

Notice from Table I that even for very high flame velocities the rate of flame area increase must also be very high if even a weak blast wave is to be generated. On the other hand, only extremely large initial flame areas, exhibiting very large flame acceleration over their entire frontal area are necessary to produce a weak blast wave from deflagrative combustion. Both of these observations imply that extremely large clouds are required if one is to produce significant overpressure by deflagrative combustion alone.

(21)

DISCUSSION AND CONCLUSIONS

The application of simple source acoustic theory to deflagrative combustion of an unconfined cloud shows that:

1) It is very difficult to produce a damaging blast wave by deflagrative combustion once the flame is not completely surrounded by a combustible mixture.

2) The maximum overpressure produced, other circumstances being equal, is proportional to the ratio of the minor dimension of the cloud to the distance to the observer.

3) Blast pressure is rather uniformly distributed in all directions, i.e., the blast is roughly spherical.

4) The cloud must be very large if a damaging blast wave is to be produced.

5) Spherical flame propagation calculations such as those of Kuhl _et al_. and Strehlow _et al_. greatly overestimate blast pressures from deflagrative combustion following edge ignition of clouds with large aspect ratios.

From various accident accounts of the sequence of events that led to the production of a damaging blast wave after delayed ignition of a massive spill of combustible material it appears that:

1. There is a threshold spill size below which blast damage does not occur. Gugan's[9] documentation of incidents shows that blast damage has been observed for spills of less than 2000 Kg but more than 100 Kg only for the fuels H_2, H_2-CO mixture, CH_4 and C_2H_4. Blast damage has been recorded only for spills greater than

2000 Kg for all other fuels.

2. In the majority of cases where blast damage occurred, fire was present for a considerable period before the blast occurred.

3. In many cases damage is highly directional.

These observations when coupled with the results of simple source acoustic theory for deflagrative combustion lead to the following conclusions.

1. There should be a size threshold below which blast will not occur as long as ignition is "soft", i.e., does not directly trigger detonation.

2. The fact that fire is present early after ignition indicates that massive flame accelerations are necessary to lead to blast wave formation. Since the flame must have burned through the cloud edge by the time the blast is produced, simple acoustic source theory must be operative for even high deflagration velocities. Thus, the blast must arise from some sort of effectively supersonic combustion process or from <u>very</u> rapid increases in effective surface area of the flame.

3. Simple acoustic source theory for deflagrative combustion shows that deflagrative processes per se cannot produce highly directional effects. However, it is well known that detonative combustion of a cloud does produce highly directional blast wave effects.

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APPENDIX A

THE GENERALIZED HEAT ADDITION HUGONIOT

Strehlow et al.[3] have shown that a generalized heat addition Hugoniot quite accurately fits the real Hugoniot for hydrocarbon-air combustion over the range of interest for vapor cloud explosions. Briefly they assume that

$$H_o = C_{p_o} T$$

and

$$h_1 = C_{p_1} T - \tilde{Q}$$

where $\tilde{Q}$ is the energy added at the deflagrative/detonative discontinuity and C_{p_o} and C_{p_1} are different heat capacities for the reactive and product gases respectively.

Using this approach they define a dimensionless energy addition as

$$\tilde{q} = (\gamma_1 - 1)\tilde{Q}/P_o V_o$$

Thus the volume change for constant pressure combustion is given by the expression

$$\frac{V_b}{V_u} = \frac{\gamma_o(\gamma_1 - 1)}{\gamma_1(\gamma_o - 1)} + \frac{\tilde{q}}{\gamma_1}$$

therefore

$$\frac{V_b - V_u}{V_u} = \frac{(\gamma_1 - \gamma_o)}{\gamma_1(\gamma_o - 1)} + \frac{\tilde{q}}{\gamma_1}$$

Now define

$$\frac{V_b - V_u}{V_u} = \frac{\hat{q}}{\gamma_o}$$

for ease of nondimensionlizing the acoustic problem. This yields

$$\hat{q} = \frac{\gamma_o(\gamma_1-\gamma_o)}{\gamma_1(\gamma_o-1)} + \frac{\gamma_o}{\gamma_1}\tilde{q}$$

For stoichiometric methane-air mixtures(3)

$$\gamma_o = 1.4 \qquad \gamma_1 = 1.202 \quad \text{and} \quad \tilde{q} = 8.430$$

Therefore

$$\frac{V_b-V_u}{V_u} = \frac{\hat{q}}{\gamma_o} = 6.6015$$

Thus $\qquad \hat{q} = 9.242$

and

$$\frac{V_b}{V_u} = 7.6015$$

for a stoichiometric methane cloud.

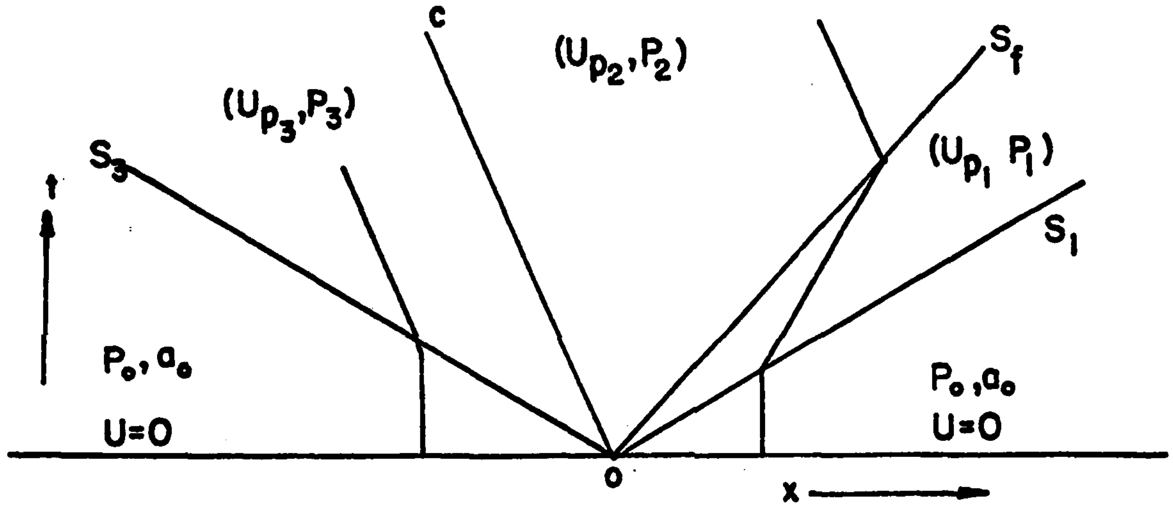

Figure 1. The wave diagram for strictly one-dimensional, constant-velocity deflagration of a free cloud after edge ignition (edge located at x = 0, S_f is apparent flame speed).

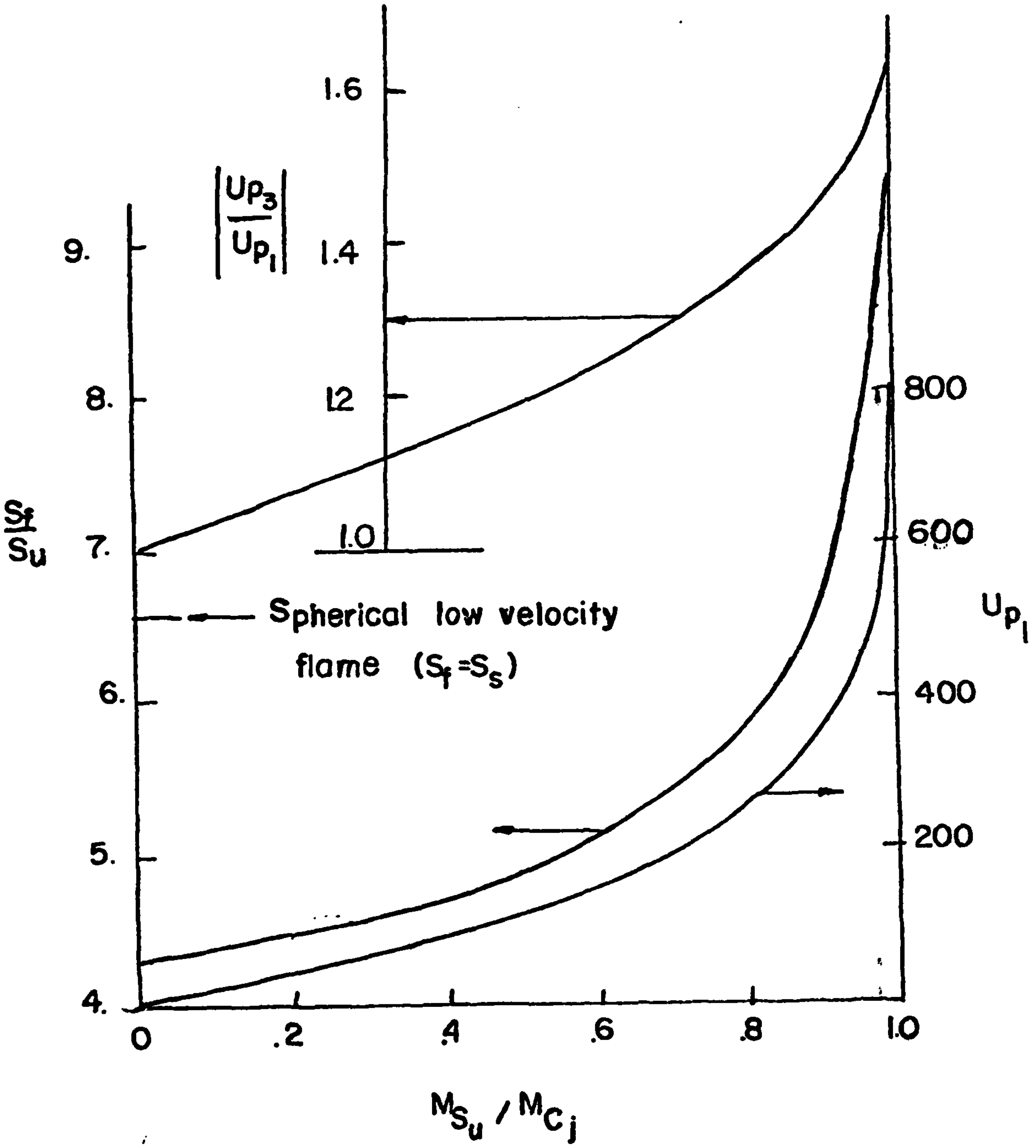

Figure 2. Flow velocities and apparent speeds associated with the strictly one-dimensional deflagration combustion illustrated in Figure 1.

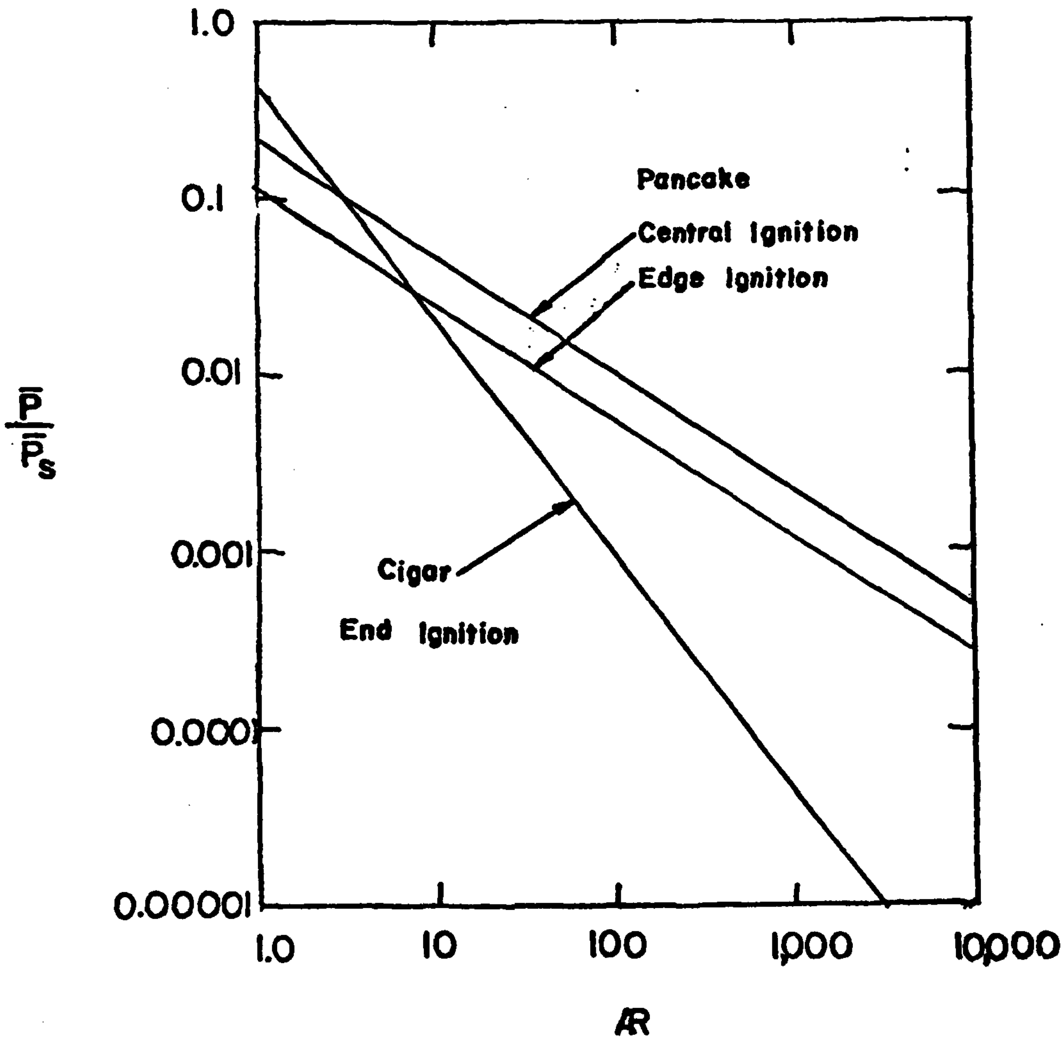

Figure 3. Effect of the aspect ratio, AR, on the maximum blast wave pressure rise for the deflagrative combustion of pancake and cigar shaped clouds. Cloud volume, normal burning velocity and observer distance from cloud center all assumed to be constant from cloud to cloud.